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YOU HAVE REQUESTED DATA FROM 3 ANSWERS - CONTINUE? Y/(N):y

L2 ANSWER 1 OF 3 CAPLUS COPYRIGHT 1997 ACS

ACCESSION NUMBER: 1994:668294 CAPLUS

DOCUMENT NUMBER: 121:268294

TITLE: Structure and absolute configuration of a monohydrate of calcipotriol, (1.alpha.,3.beta.,5Z,7E,22E,24S)-24-cyclopropyl-9,10-secochola-5,7,10(19),22-tetraene-1,3,24-triol. [Erratum to document cited in CA118(24):245113x]

AUTHOR(S): Larsen, Sine; Hansen, Erik T.; Hoffmeyer, lene; Rastrup-Andersen, Niels

CORPORATE SOURCE: Dep. Chem., Univ. Copenhagen, Copenhagen, DK-2100, Den.

SOURCE: Acta Crystallogr., Sect. C: Cryst. Struct. Commun. (1993), C49(12), 2184  
CODEN: ACSCEE; ISSN: 0108-2701

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The errors were reflected in the abstr.

IT 147657-22-5

RL: PRP (Properties)

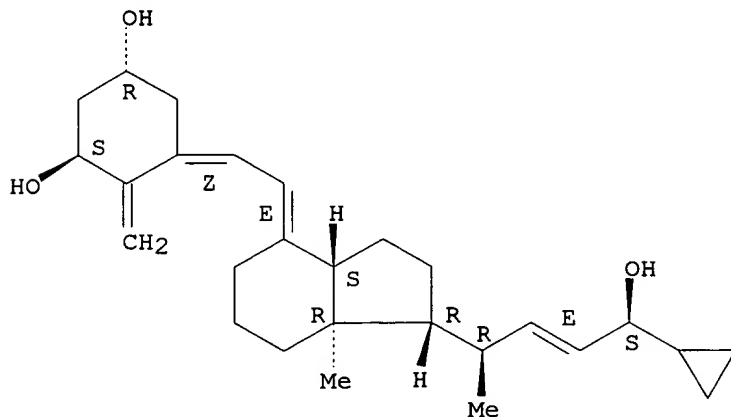
(crystal structure and abs. configuration of (Erratum))

RN 147657-22-5 CAPLUS

CN 9,10-Secochole-5,7,10(19),22-tetraene-1,3,24-triol, 24-cyclopropyl-, monohydrate, (1.alpha.,3.beta.,5Z,7E,22E,24S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.



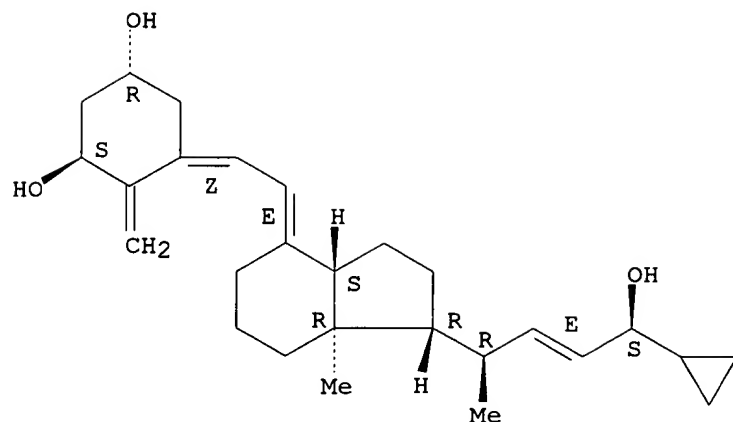
● H<sub>2</sub>O

L2 ANSWER 2 OF 3 CAPLUS COPYRIGHT 1997 ACS

ACCESSION NUMBER: 1994:631161 CAPLUS  
DOCUMENT NUMBER: 121:231161  
TITLE: Preparation and formulation of calcipotriol hydrate  
INVENTOR(S): Hansen, Erik Torngaard; Rastrup, Andersen Niels Smidt; Ringborg, Lene Hoffmeyer  
PATENT ASSIGNEE(S): Leo Pharmaceutical Products Ltd. a/s, Den.  
SOURCE: PCT Int. Appl., 10 pp.  
CODEN: PIXXD2

	NUMBER	DATE
PATENT INFORMATION:	WO 9415912 A1	940721
DESIGNATED STATES:	W: AU, BB, BG, BR, BY, CA, CN, CZ, FI, HU, JP, KP, KR, KZ, LK, LV, MG, MN, MW, NO, NZ, PL, RO, RU, SD, SK, UA, US, UZ, VN RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG	
APPLICATION INFORMATION:	WO 94-DK11	940107
PRIORITY APPLN. INFO.:	GB 93-763	930115
DOCUMENT TYPE:	Patent	
LANGUAGE:	English	
AB	The present invention relates to calcipotriol hydrate, a new cryst. form of calcipotriol, with superior tech. properties and with superior stability.	
IT	<b>147657-22-5P</b> RL: BAC (Biological activity or effector, except adverse); IMF (Industrial manufacture); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (prepn. and formulation of new crystn. form)	
RN	147657-22-5 CAPLUS	
CN	9,10-Secochola-5,7,10(19),22-tetraene-1,3,24-triol, 24-cyclopropyl-, monohydrate, (1.alpha.,3.beta.,5Z,7E,22E,24S)- (9CI) (CA INDEX NAME)	

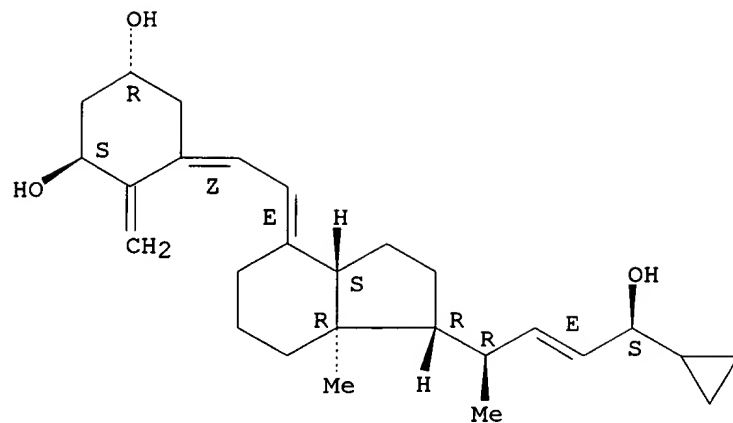
Absolute stereochemistry.  
Double bond geometry as shown.



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L2 ANSWER 3 OF 3 CAPLUS COPYRIGHT 1997 ACS  
 ACCESSION NUMBER: 1993:245113 CAPLUS  
 DOCUMENT NUMBER: 118:245113  
 TITLE: Structure and absolute configuration of a monohydrate of calcipotriol, (1.alpha.,3.beta.,5Z,7E,22E,24S)-24-cyclopropyl-9,10-secochola-5,7,10(19),22-tetraene-1,3,24-triol  
 AUTHOR(S): Larsen, Sine; Hansen, Erik T.; Hoffmeyer, Lene; Rastrup-Andersen, Niels  
 CORPORATE SOURCE: Dep. Chem., Univ. Copenhagen, Copenhagen, DK-2100, Den.  
 SOURCE: Acta Crystallogr., Sect. C: Cryst. Struct. Commun. (1993), C49(3), 618-21  
 CODEN: ACSCEE; ISSN: 0108-2701  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB The title compd. is monoclinic, space group P2<sub>1</sub>, with a 9.4377(10), b 6.9780(11), c 18.559(3) .ANG., and .beta. 93.240(13).degree.; Z = 2, dc = 1.172; R = 0.050, Rw = 0.064 for 3913 reflections. At. coordinates are given. The abs. configuration of calcipotriol was established to be 1S,3R,8R,14S,17R,20S,24S. The mol. geometry of calcipotriol is similar to the stereochem. obsd. in the structures of the related D vitamins.  
 IT **147657-22-5**, Calcipotriol monohydrate  
 RL: PRP (Properties)  
 (crystal structure and abs. configuration of)  
 RN 147657-22-5 CAPLUS  
 CN 9,10-Secochole-5,7,10(19),22-tetraene-1,3,24-triol, 24-cyclopropyl-, monohydrate, (1.alpha.,3.beta.,5Z,7E,22E,24S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.  
 Double bond geometry as shown.



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(FILE 'HOME' ENTERED AT 11:58:32 ON 19 NOV 1997)

L1 FILE 'REGISTRY' ENTERED AT 11:58:51 ON 19 NOV 1997  
1 S CALCIPOTRIOL MONOHYDRATE/CN

L2 FILE 'CAPLUS' ENTERED AT 11:59:17 ON 19 NOV 1997  
3 S L1

L3 FILE 'USPATFULL' ENTERED AT 12:00:13 ON 19 NOV 1997  
0 S L1